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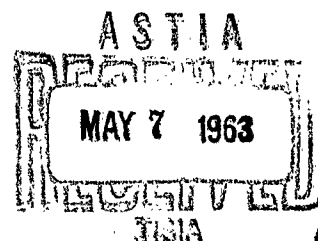
## THE SPM METHOD FOR NEUTRONS

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J. Heitner, authors.)

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## FOREWORD

This report was prepared by TRG, Incorporated, Syosset, N. Y. under USAF Contract No. AF 33(616)-7732. The contract was initiated under Project No. 7360, "The Chemistry and Physics of Materials," Task No. 736003, "Interaction of High Energy Forms with Materials." The work was administered under the direction of the Directorate of Materials and Processes, Deputy for Technology, Aeronautical Systems Division, Wright-Patterson Air Force Base, Ohio. Lt. W. H. Dyke directed the work with Mr. V. L. Donlan acting as project engineer.

This report covers work done from 15 December 1960 to 15 April 1962.

This program was initially under the supervision of C. N. Klahr and subsequently under supervision of R. Aronson.

## ABSTRACT

The SPM equation has been recoded for the IBM-7090.  
Both theoretical analysis and some numerical results are given  
and discussed.

This technical documentary report has been reviewed and is  
approved.



RICHARD J. VOSSLER Capt, USAF  
Chief, Radiation Branch  
Physics Laboratory  
Directorate of Materials & Processes

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## I. Introduction

The aim of the present program was to program the Stochastic Process Method (SPM)<sup>1</sup> for neutron problems and to investigate the method both theoretically and numerically. We have been able to analyze the problem sufficiently to determine proper source and interface conditions, as well as appropriate methods of treating scattering by hydrogen and inelastic scattering by heavy elements within the spirit of the method.

In this report are presented the SPM equations with boundary conditions, a discussion of some of the results, and operating instructions for the IBM-7090 SPM code and for the auxiliary input code GENUC.

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## II. Analysis of the SPM Equation

### A. Primitive SPM Equation for Variable Cross-Sections

An SPM equation can be derived for cross sections which vary in space and energy. The previous derivation was valid only for constant cross sections. We now derive the new result.

The integral Boltzmann equation can be written

$$\begin{aligned} \sigma(x,u)\phi(x,u) = & \psi_0(x,u) + 2\pi \int_{-\infty}^{\infty} dx' \int_0^u du' \int_{-1}^1 d\mu \int_{-1}^1 d\mu' \frac{\sigma(x,u)}{|\mu|} H\left(\frac{x-x'}{\mu}\right) \\ & \times \exp\left\{-\frac{1}{\mu} \int_{x'}^x \sigma(x'',u) dx''\right\} \int_{-1}^1 dv \int_0^{2\pi} d\phi \delta[u-u'-L(v)] \times \\ & \times \delta(\mu-\mu'v - \sqrt{1-\mu'^2} \sqrt{1-v^2} \cos\phi) \sigma_s(x',u',v) \phi'(x',u',\mu'). \quad (1) \end{aligned}$$

Here

$x$  = distance from source plane

$u$  = lethargy

$\mu$  = cosine of angle with normal to source plane

$v$  = cosine of scattering angle

$\phi'$  = azimuthal angle of scattering

$\sigma(x,u)$  = total macroscopic cross section at  $x$  and  $u$

$\sigma_s(x,u,v)$  = macroscopic differential elastic scattering

cross section at  $x$  and  $u$  for scattering through an angle

whose cosine is  $v$ , per unit solid angle

$\phi(x,u,\mu)$  = flux at  $(x,u,\mu)$  per unit lethargy and solid angle



$L(v)$  = increase in lethargy accompanying scattering through an angle whose cosine is  $v$

$\psi_0(x,u)$  = density of first collisions at  $x$  and  $u$  per unit volume, time, and lethargy

Primed variables refer to the situation before collision.

Also,  $\phi(x,u)$  is the total flux at  $x$  and  $u$  per unit lethargy:

$$\phi(x,u) = 2\pi \int_{-1}^1 \phi(x,u,\mu) d\mu \quad (2)$$

and  $H(\xi)$  is a step function:

$$\begin{aligned} H(\xi) &= 1, & \xi > 0 \\ &= 0, & \xi < 0. \end{aligned} \quad (3)$$

Let the total number of mean free paths at lethargy  $u$  between 0 and  $x$  be

$$s(x,u) = \int_0^x \sigma(x'',u) du''. \quad (4)$$

$s$  is thus a function of  $x$  with parameter  $u$  and conversely,  $x$  is a function of  $s$ . We will also use the notation

$$s' = s(x', u). \quad (5)$$

Let

$$\frac{\sigma_s(x',u',v)}{\sigma_s(x',u)} \phi(x',u',\mu') = f(x'(s'), u',u,v,\mu') = g(s'). \quad (6)$$

By Taylor's expansion,

$$g(s') = \sum_{n=0}^{\infty} \frac{1}{n!} (s'-s)^n \frac{\partial^n}{\partial s^n} g(s), \quad (7)$$

where by (6),

$$g(s) = f(x(s), u', u, v, \mu') = \frac{\sigma_s(x, u', v)}{\sigma_s(x, u)} \phi(x, u', \mu'). \quad (8)$$

We have also

$$H\left(\frac{x-x'}{\mu}\right) = H\left(\frac{s-s'}{\mu}\right). \quad (9)$$

Then the  $x'$  - integral in (1) can be written

$$\begin{aligned} & \int_{-\infty}^{\infty} \frac{\sigma(x, u)}{|\mu|} H\left(\frac{x-x'}{\mu}\right) \exp\left\{-\frac{1}{\mu} \int_{x'}^x \sigma(x'', u) dx''\right\} \sigma_s(x', u, v) \phi(x', u', \mu') dx' = \\ &= \sigma(x, u) \int_{-\infty}^{\infty} dx' \frac{\sigma(x', u)}{|\mu|} H\left(\frac{s-s'}{\mu}\right) e^{-\frac{s-s'}{\mu} \frac{\sigma_s(x', u, v)}{\sigma_s(x', u)}} \phi(x', u', \mu') = \\ &= \sigma(x, u) \sum_{n=0}^{\infty} \frac{1}{n!} \int_{-\infty}^{\infty} \frac{ds'}{|\mu|} H\left(\frac{s-s'}{\mu}\right) e^{-\frac{s-s'}{\mu}} (s'-s)^n \frac{\partial^n}{\partial s^n} g(s) = \\ &= \sum_{n=0}^{\infty} (-1)^n \mu^n \sigma(x, u) \frac{\partial^n}{\partial s^n} g(s). \end{aligned} \quad (10)$$

The second equality in (10) holds by virtue of (4), (6), (7), and (9). But by (4),

$$\frac{\partial}{\partial s} = \frac{1}{\sigma(x, u)} \frac{\partial}{\partial x}, \quad (11)$$

so

$$\begin{aligned} \sigma(x, u) \frac{\partial^n}{\partial s^n} g(s) &= \sigma(x, u) \left[ \frac{1}{\sigma(x, u)} \frac{\partial}{\partial x} \right]^n \frac{\sigma(x, u', v)}{\sigma(x, u)} \phi(x, u', \mu') = \\ &= \left[ \frac{\partial}{\partial x} \frac{1}{\sigma(x, u)} \right]^n \sigma_s(x, u', v) \phi(x, u', \mu'). \end{aligned} \quad (12)$$

Inserting (12) into (10) and then (10) into (1), we have

$$\begin{aligned} \sigma(x, u) \phi(x, u) &= \psi_0(x, u) + 2\pi \sum_{n=0}^{\infty} (-1)^n \int_{-1}^1 d\mu' \int_{-1}^1 dv \int_0^{2\pi} d\phi' \int_{-1}^1 d\mu'' \int_0^u du' \times \\ &\times \left[ \frac{\partial}{\partial x} \frac{1}{\sigma(x, u)} \right]^n \mu^n \delta(\mu - \mu' v - \sqrt{1 - \mu'^2} \sqrt{1 - v'^2} \cos \phi) \delta[u - u' - L(v)] \times \\ &\times \sigma_s(x, u', v) \phi(x, u', \mu'). \end{aligned} \quad (13)$$

We now expand  $\sigma\phi$  about  $u$ :

$$\sigma_s(x, u', v) \phi(x, u', \mu') = \sum_{m=0}^{\infty} \frac{1}{m!} (u' - u)^m \frac{\partial^m}{\partial u^m} \frac{\sigma_s(x, u, v)}{\sigma_s(x, u)} \sigma_s(x, u) \phi(x, u) M(\mu' | x, u) \quad (14)$$

where  $\sigma_s(x, u)$  is the elastic scattering cross section at  $x$  and  $u$ :

$$\sigma_s(x, u) = 2\pi \int_{-1}^1 \sigma_s(x, u, v) dv \quad (15)$$

and

$$M(\mu' | x, u) = \frac{\phi(x, u, \mu')}{\phi(x, u)}. \quad (16)$$

Inserting (14) into (13), integrating over  $u'$  and  $\mu$ , and then dropping the prime on  $\mu'$ , we have the SPM equation:

$$\begin{aligned} \sigma(x, u) &= \psi_0(x, u) + \\ &+ \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{(-1)^{m+n}}{m!} \left[ \frac{\partial}{\partial x} \frac{1}{\sigma(x, u)} \right]^n \frac{\partial^m}{\partial u^m} C_{mn}(x, u) \phi(x, u), \end{aligned} \quad (17)$$

where

$$C_{mn}(x, u) = 2\pi \int_{-1}^1 M(\mu | x, u) d\mu \int_{-1}^1 L^m(v) \frac{\sigma_s(x, u, v)}{\sigma_s(x, u)} dv \int_0^{2\pi} [\mu v + \sqrt{1-\mu^2} \sqrt{1-v^2} \cos \phi]^n d\phi. \quad (18)$$

Equations (17) and (18) are precisely the same relations as for constant cross sections, except that now we must make sure that the  $\sigma(x, u)$  are placed as given in (17), since  $\sigma$  no longer commutes with the derivatives.

If the medium consists of a number of nuclides, each has its own  $C_{mn}$ . The appropriate generalization retains eq. (17) with  $C_{mn}$  defined by the relation

$$C_{mn} \sigma_s = \sum_i C_{mn}^i \sigma_s^i, \quad (19)$$

where

$$\begin{aligned} \sigma_s^i &= \text{macroscopic scattering cross section for } i^{\text{th}} \text{ nuclide} \\ \sigma_s &= \sum_i \sigma_s^i \end{aligned}$$

and  $C_{mn}^i$  is defined by eq. (19) with the cross sections  $\sigma_s^i$  being used.

Note that  $C_{00} = 1$ .

#### B. The Truncated SPM Equation and the Expression for the Current

To second order in both  $x$  and  $u$ , the SPM equation (17) reduces in the absence of a source  $\psi_0$  to

$$\begin{aligned} & - (\sigma - \sigma_s) \phi - \frac{\partial}{\partial u} C_{10} \sigma_s \phi + \frac{1}{2} \frac{\partial^2}{\partial u^2} C_{20} \sigma_s \phi - \frac{\partial}{\partial x} \frac{1}{\sigma} C_{01} \sigma_s \phi + \frac{\partial}{\partial x} \frac{1}{\sigma} \frac{\partial}{\partial x} \frac{1}{\sigma} C_{02} \sigma_s \phi + \\ & + \frac{\partial}{\partial x} \frac{1}{\sigma} \frac{\partial}{\partial u} C_{11} \sigma_s \phi - \frac{\partial}{\partial x} \frac{1}{\sigma} \frac{\partial}{\partial x} \frac{1}{\sigma} \frac{\partial}{\partial u} C_{12} \sigma_s \phi - \frac{1}{2} \frac{\partial}{\partial x} \frac{1}{\sigma} \frac{\partial^2}{\partial u^2} C_{21} \sigma_s + \\ & + \frac{1}{2} \frac{\partial}{\partial x} \frac{1}{\sigma} \frac{\partial}{\partial x} \frac{1}{\sigma} \frac{\partial^2}{\partial u^2} C_{22} \sigma_s \phi = 0 \end{aligned} \quad (20)$$

It was shown in the original summary report<sup>1</sup> that the current J obeys the equation

$$-\frac{\partial J}{\partial x} = \sum_{m=0}^{\infty} \sum_{n=1}^{\infty} \frac{(-1)^{m+n}}{m!} \left[ \frac{\partial}{\partial x} \frac{1}{\sigma(x,u)} \right]^n \frac{\partial^m}{\partial u^m} C_{mn} \sigma_s \phi, \quad (21)$$

where we have used the general form (17) of the SPM equation.

In the order to which we are truncating, we can then write

$$J = -\frac{1}{\sigma} \left[ -C_{01} + \frac{\partial}{\partial x} \frac{1}{\sigma} C_{02} + \frac{\partial}{\partial u} C_{11} - \frac{\partial}{\partial x} \frac{1}{\sigma} \frac{\partial}{\partial u} C_{12} - \frac{1}{2} \frac{\partial^2}{\partial u^2} C_{21} + \frac{1}{2} \frac{\partial}{\partial x} \frac{1}{\sigma} \frac{\partial^2}{\partial u^2} C_{22} \right] \sigma_s \phi. \quad (22)$$

Now let

$$C_{m1} \frac{\sigma_s}{\sigma} = v_m \langle \mu \rangle = v_m \frac{J}{\phi}. \quad (23)$$

$v_m$  is defined here somewhat differently from the way in which it was defined previously.<sup>1</sup>

Then

$$\begin{aligned} & - (1-v_0) J - \frac{1}{\sigma} \frac{\partial}{\partial u} (v_1 \sigma J) + \frac{1}{2\sigma} \frac{\partial^2}{\partial u^2} (v_2 \sigma J) = \\ & = \frac{1}{\sigma} \frac{\partial}{\partial x} \frac{1}{\sigma} \left[ C_{02} \sigma_s \phi - \frac{\partial}{\partial u} (C_{12} \sigma_s \phi) + \frac{1}{2} \frac{\partial^2}{\partial u^2} (C_{22} \sigma_s \phi) \right]. \end{aligned} \quad (24)$$

Suppose that successively higher u-derivatives correspond to successively higher powers of some small parameter  $\lambda$ . Thus if some quantity f is of order unity  $[O(1)]$

$$\frac{\partial^n f}{\partial u^n} = O(\lambda^n)$$

Expand J in orders of  $\lambda$  such that  $J_n = O(\lambda^n)$ . Then to second order,

$$J = J_0 + J_1 + J_2. \quad (25)$$

Again to second order, (24) becomes

$$\begin{aligned}
 & -(1-v_o)(J_o + J_1 + J_2) - \frac{1}{\sigma} \frac{\partial}{\partial u} (v_1 \sigma J_o + v_1 \sigma J_1) + \frac{1}{2\sigma} \frac{\partial^2}{\partial u^2} (v_2 \sigma J_o) = \\
 & = \frac{1}{\sigma} \frac{\partial}{\partial x} \frac{1}{\sigma} \left[ C_{02} \sigma_s \theta - \frac{\partial}{\partial u} (C_{12} \sigma_s \theta) + \frac{1}{2} \frac{\partial^2}{\partial u^2} (C_{22} \sigma_s \theta) \right]. \quad (26)
 \end{aligned}$$

Then

$$-(1-v_o)J_o = \frac{1}{\sigma} \frac{\partial}{\partial x} \frac{1}{\sigma} C_{02} \sigma_s \theta \quad (27)$$

$$-(1-v_o)J_1 - \frac{1}{\sigma} \frac{\partial}{\partial u} (v_1 \sigma J_o) = - \frac{1}{\sigma} \frac{\partial}{\partial x} \frac{1}{\sigma} \frac{\partial}{\partial u} C_{12} \sigma_s \theta \quad (28)$$

$$-(1-v_o)J_2 - \frac{1}{\sigma} \frac{\partial}{\partial u} (v_1 \sigma J_1) + \frac{1}{2\sigma} \frac{\partial^2}{\partial u^2} (v_2 \sigma J_o) = \frac{1}{\sigma} \frac{\partial}{\partial x} \frac{1}{\sigma} \frac{\partial^2}{\partial u^2} C_{22} \sigma_s \theta. \quad (29)$$

From eqs. (27)-(29), we get

$$J_o = - \frac{1}{1-v_o} \frac{1}{\sigma} \frac{\partial}{\partial x} \frac{1}{\sigma} C_{02} \sigma_s \theta \quad (30)$$

$$J_1 = \frac{1}{1-v_o} \frac{1}{\sigma} \left[ \frac{\partial}{\partial x} \frac{1}{\sigma} \frac{\partial}{\partial u} C_{12} \sigma_s \theta + \frac{\partial}{\partial u} \frac{v_1}{1-v_o} \frac{\partial}{\partial x} \frac{1}{\sigma} C_{02} \sigma_s \theta \right] \quad (31)$$

$$\begin{aligned}
 J_2 = & - \frac{1}{1-v_o} \frac{1}{\sigma} \left[ \frac{\partial}{\partial x} \frac{1}{\sigma} \frac{\partial^2}{\partial u^2} C_{22} \sigma_s \theta + \frac{1}{2} \frac{\partial^2}{\partial u^2} \frac{v_2}{1-v_o} \frac{\partial}{\partial x} \frac{1}{\sigma} C_{02} \sigma_s \theta + \right. \\
 & \left. + \frac{\partial}{\partial u} \frac{v_1}{1-v_o} \left\{ \frac{\partial}{\partial x} \frac{1}{\sigma} \frac{\partial}{\partial u} C_{12} \sigma_s \theta + \frac{\partial}{\partial u} \frac{v_1}{1-v_o} \frac{\partial}{\partial x} \frac{1}{\sigma} C_{02} \sigma_s \theta \right\} \right] \quad (32)
 \end{aligned}$$

Only for constant cross sections can expressions (30)-(32) be combined to give a current of the form

$$J = - \frac{1}{\sigma} \frac{\partial}{\partial x} \left[ \beta_1 \sigma_s \theta + \frac{\partial}{\partial u} \beta_2 \sigma_s \theta + \frac{\partial^2}{\partial u^2} \beta_3 \sigma_s \theta \right] \quad (33)$$

In the general case, we must use eqs. (25), (30), (31), and (32) to give the expression for J. J is, of course, taken to be continuous. We obtain the truncated SPM equation in the form

$$- \alpha_0 \phi - \frac{\partial}{\partial u} \alpha_1 \phi + \frac{\partial^2}{\partial u^2} \alpha_2 \phi - \frac{\partial J}{\partial x} = 0 \quad (34)$$

where

$$\alpha_0 = \sigma - \sigma_s \quad (35a)$$

$$\alpha_1 = C_{10} \sigma_s \quad (35b)$$

$$\alpha_2 = \frac{1}{2} C_{20} \sigma_s. \quad (35c)$$

Because the  $J_2$  term was found not to improve the results, the approximation was actually cut off after  $J_1$ .

### C. Interface Conditions

The conditions at an interface must be continuity of  $\phi$  and  $J$ , for all lethargies. It is necessary to see how this works out in a difference approximation.

We assume an interface at  $x = 0$ . Then

$$-\alpha_0 \phi - \frac{\partial}{\partial u} \alpha_1 \phi + \frac{\partial^2}{\partial u^2} \alpha_2 \phi - \frac{\partial J}{\partial x} = 0, \quad x \neq 0 \quad (36)$$

We will denote the value of  $J$  at the interface by  $J_0$ . If  $\delta_+$  is the  $x$ -interval to the first mesh point to the right of the interface and  $\delta_-$  that to the mesh point to the left, we have

$$J_0 = J_- + \delta_- J'_-, \quad (37)$$

where

$J_-$  = value of  $J$  at the first mesh point to the left

$J'_-$  = average value of  $\frac{\partial J}{\partial x}$  in left-hand interval.

The mean value of  $J$  in the left-hand interval is

$$\bar{J}_- = \frac{1}{2} (J_0 + J_-). \quad (38)$$

Then

$$-J'_- = \frac{J_- - J_0}{\delta_-} = \frac{2}{\delta_-} (\bar{J}_- - J_0) \quad (39)$$

Similarly,

$$-J'_+ = \frac{2}{\delta_+} (J_0 - J_+). \quad (40)$$



If  $\alpha_{i+}$  is the value of  $\alpha_i$  to the right of the interface and  $\alpha_{i-}$  that to the left, we have

$$-\delta_{-}\alpha_{0-}\theta - \frac{\partial}{\partial u} \delta_{-}\alpha_{1-}\theta + \frac{\partial^2}{\partial u^2} \delta_{-}\alpha_{2-}\theta + 2(\bar{J}_{-} - J_0) = 0 \quad (41a)$$

$$-\delta_{+}\alpha_{0+}\theta - \frac{\partial}{\partial u} \delta_{+}\alpha_{1+}\theta + \frac{\partial^2}{\partial u^2} \delta_{+}\alpha_{2+}\theta + 2(J_0 - \bar{J}_{+}) = 0 \quad (41b)$$

Defining

$$\alpha_i = \frac{\delta_{+}\alpha_{i+} + \delta_{-}\alpha_{i-}}{\delta_{+} + \delta_{-}} \quad (42)$$

and adding the two equations (41 a,b) we have

$$-\alpha_0\theta - \frac{\partial}{\partial u} \alpha_1\theta + \frac{\partial^2}{\partial u^2} \alpha_2\theta + \frac{2}{\delta_{+} + \delta_{-}} (\bar{J}_{-} - \bar{J}_{+}) = 0 \quad (43)$$

Equation (43) is precisely what we have within a single medium.

Thus we can treat boundary points the same as any other points if we define the  $\alpha_i$  at the boundary by eq. (42). The cross section-dependent constants in  $\bar{J}_{+}$  are those appropriate to the right-hand medium and those in  $\bar{J}_{-}$  are those appropriate to the left-hand medium. We can write

$$J = -\gamma_3 \left[ \frac{\partial}{\partial x} \alpha_3\theta - \frac{\partial}{\partial x} \gamma_4 \frac{\partial}{\partial u} \alpha_4\theta - \frac{\partial}{\partial u} \gamma_5 \frac{\partial}{\partial x} \alpha_3\theta \right], \quad (44)$$

where

$$\begin{aligned} \gamma_3 &= \frac{1}{1-v_0} \frac{1}{\sigma} & \alpha_3 &= \frac{1}{\sigma} C_{02}\sigma_s \\ \gamma_4 &= \frac{1}{\sigma} & \alpha_4 &= C_{12}\sigma_s \\ \gamma_5 &= \frac{v_1}{1-v_0} \end{aligned} \quad (45)$$

Then in our difference approximation

$$\bar{J}_+ = \bar{J}_+ \gamma_{3\pm} \left\{ + \frac{\alpha_{3\pm} \phi_{\pm 1} - \alpha_{3\pm} \phi_0}{\delta_{\pm}} - \frac{\gamma_{4\pm} \frac{\partial}{\partial u} \alpha_{4\pm} \phi_{\pm 1} - \gamma_{4\pm} \frac{\partial}{\partial u} \alpha_{4\pm} \phi_0}{\delta_{\pm}} - \frac{\partial}{\partial u} \gamma_{5\pm} \frac{\alpha_{3\pm} \phi_{\pm 1} - \alpha_{3\pm} \phi_0}{\delta_{\pm}} \right\}, \quad (46)$$

where

$$\begin{aligned} \phi_0 &= \phi(x = 0) \\ \phi_{\pm 1} &= \phi(x \pm \delta_{\pm}). \end{aligned} \quad (47)$$

Expression (46) is to be substituted into eq. (43).

Note that  $\bar{J}$  is not assumed continuous across the boundary  $\bar{J}_+ - \bar{J}_- \rightarrow 0$  for  $\delta_+ \rightarrow 0$ ,  $\delta_- \rightarrow 0$ , but for a finite mesh, we do not use the continuity of  $J$  as an explicit condition.

#### D. The Constants $C_{mn}$

We had

$$C_{mn}(x, u) = 2\pi \int_{-1}^1 M(\mu|x, u) d\mu \int_{-1}^1 L^m(v) \frac{\sigma_s(x, u, v)}{\sigma_s(x, u)} dv \int_0^{2\pi} [\mu v + \sqrt{1-\mu^2} \sqrt{1-v^2} \cos \phi]^n d\phi. \quad (18)$$

We assume that within a given medium  $C_{mn}$  is independent of  $x$  and further, that  $M(\mu|x, u)$  is independent of  $u$ .

Let

$$\nu = \mu v + \sqrt{1-\mu^2} \sqrt{1-v^2} \cos \phi \quad (48)$$

We can expand

$$\nu^n = \sum_{l=0}^n b_{nl} P_l(\nu). \quad (49)$$

Then

$$\begin{aligned}
 \int_0^{2\pi} \nu^n d\phi &= \sum_{\ell=0}^n b_{n\ell} \int_0^{2\pi} P_\ell(\nu) d\phi = \\
 &= \sum_{\ell=0}^n b_{n\ell} \int_0^{2\pi} \left[ P_\ell(\mu) P_\ell(\nu) + 2 \sum_{m=0}^{\ell} P_\ell^m(\nu) \cos m\phi \right] d\phi = \\
 &= 2\pi \sum_{\ell=0}^n b_{n\ell} P_\ell(\mu) P_\ell(\nu). \tag{50}
 \end{aligned}$$

The second equality arises from the addition theorem for Legendre Polynomials.

We use also the inverse of (47):

$$P_\ell(\mu) = \sum_{k=0}^{\ell} a_k \mu^k \tag{51}$$

and define

$$\langle \mu^n \rangle = 2\pi \int_{-1}^1 M(\mu) \mu^n d\mu. \tag{52}$$

The differential cross section as a function of the cosine  $\omega$  of the scattering angle in the center-of-mass system is expanded as

$$\sigma_s(u, \omega) = \frac{\sigma_s(u)}{4\pi} \sum_{\ell=0}^{\infty} (2\ell+1) f_\ell(u) P_\ell(\omega), \tag{53}$$

where  $\sigma_s(u)$  is the total macroscopic scattering cross section at  $u$ , from which it follows that  $f_0(u) = 1$ . The relation between  $\nu$  and  $\omega$  is such that

$$\sigma_s(u, \nu) d\nu = \sigma_s(u, \omega) d\omega. \tag{54}$$

Thus we can write

$$C_{mn} = \int_{-1}^1 M(\mu) d\mu \int_{-1}^1 L^m(v) \frac{1}{4\pi} \sum_{\ell=0}^{\infty} (2\ell+1) f_{\ell}(u) P_{\ell}(\omega) d\omega 2\pi \sum_{r=0}^n f_{nr} \sum_{k=0}^r a_{rk} \mu_k^r \sum_{p=0}^r a_{rp} v^p =$$

$$= \frac{1}{2} \sum_{\ell=0}^{\infty} (2\ell+1) f_{\ell}(u) \sum_{r=0}^n b_{nr} \sum_{p=0}^r a_{rp} \sum_{k=0}^r a_{rk} \langle \mu^k \rangle J_{\ell pm}, \quad (55)$$

where

$$J_{\ell pm} = \int_{-1}^1 L^m(v) v^p P_{\ell}(\omega) d\omega. \quad (56)$$

For hydrogen the lower limit of the integral over  $\omega$  is zero.

We can write

$$C_{m0} = \frac{1}{2} \sum_{\ell=0}^{\infty} (2\ell+1) f_{\ell} J_{\ell 0m} \quad (57)$$

$$v_m = \frac{1}{2} \sum_{\ell=0}^{\infty} (2\ell+1) f_{\ell} J_{\ell 1m} \quad (58)$$

$$C_{m2} = \frac{\langle \mu^2 \rangle}{2} \sum_{\ell=0}^{\infty} (2\ell+1) f_{\ell} \frac{3J_{\ell 2m} - J_{\ell 0m}}{2} + \frac{1}{2} \sum_{\ell=0}^{\infty} (2\ell+1) f_{\ell} \frac{J_{\ell 0m} - J_{\ell 2m}}{2}$$

$$= \frac{1 - \langle \mu^2 \rangle}{2} C_{m0} + \frac{3\langle \mu^2 \rangle - 1}{2} \sum_{\ell=0}^{\infty} \left(\ell + \frac{1}{2}\right) f_{\ell} J_{\ell 2m} \quad (59)$$

The sum over  $\ell$  actually will be cut off at some value  $\ell = L$ . For an isotropic flux,  $\langle \mu^2 \rangle = \frac{1}{3}$  and

$$C_{m2} = \frac{1}{3} C_{m0} \quad (59a)$$

$J_{\ell pm}$  is evaluated recursively in the code

### E. The Calculation Method

We use three-point difference approximation formulas for both first and second derivatives. For the first derivative we have a weighted average of the forward and backward derivatives, thus:

$$\begin{aligned} \left. \frac{\partial \phi}{\partial u} \right|_k &= \left( \frac{1}{\Delta_+} + \frac{1}{\Delta_-} \right)^{-1} \left[ \frac{1}{\Delta_+} \frac{\phi_{k+1} - \phi_k}{\Delta_+} + \frac{1}{\Delta_-} \frac{\phi_k - \phi_{k-1}}{\Delta_-} \right] \\ &= \frac{1}{\Delta_+ + \Delta_-} \left[ \frac{\Delta_-}{\Delta_+} \phi_{k+1} + \left( \frac{\Delta_+}{\Delta_-} - \frac{\Delta_-}{\Delta_+} \right) \phi_k - \frac{\Delta_+}{\Delta_-} \phi_{k-1} \right], \end{aligned} \quad (60)$$

where

$$\left. \frac{\partial \phi}{\partial u} \right|_k = \text{value of } \frac{\partial \phi}{\partial u} \text{ at } u_k.$$

$$\phi_k = \phi(u_k)$$

$$\Delta_+ = u_{k+1} - u_k$$

$$\Delta_- = u_k - u_{k-1}$$

For the second derivative we take a difference quotient between the forward and backward first differences:

$$\begin{aligned} \left. \frac{\partial^2 \phi}{\partial u^2} \right|_k &= \left( \frac{\Delta_+ + \Delta_-}{2} \right)^{-1} \left[ \frac{\phi_{k+1} - \phi_k}{\Delta_+} - \frac{\phi_k - \phi_{k-1}}{\Delta_-} \right] \\ &= \frac{2}{\Delta_+ + \Delta_-} \left[ \frac{1}{\Delta_+} \phi_{k+1} - \left( \frac{1}{\Delta_+} + \frac{1}{\Delta_-} \right) \phi_k + \frac{1}{\Delta_-} \phi_{k-1} \right] \end{aligned} \quad (61)$$

Suppose  $\phi_{jk}$  is the flux at position mesh point  $j$  and lethargy mesh point  $k$ . Let us define

$$\begin{aligned}
\eta_+ &= \frac{\Delta_-}{\Delta_+(\Delta_+ + \Delta_-)} & \eta_- &= -\frac{\Delta_+}{\Delta_-(\Delta_+ + \Delta_-)} \\
\mu_+ &= \frac{2}{\Delta_+(\Delta_+ + \Delta_-)} & \mu_- &= \frac{2}{\Delta_-(\Delta_+ + \Delta_-)} \\
\lambda_+ &= \frac{2}{\delta_+(\delta_+ + \delta_-)} & \lambda_- &= \frac{2}{\delta_-(\delta_+ + \delta_-)}
\end{aligned} \tag{62}$$

where

$$\delta_+ = x_{j+1} - x_j$$

$$\delta_- = x_j - x_{j-1}$$

Then

$$\left. \frac{\partial \phi}{\partial u} \right|_{jk} = \eta_+ \phi_{j,k+1} - (\eta_+ + \eta_-) \phi_{jk} + \eta_- \phi_{j,k-1} \tag{63a}$$

$$\left. \frac{\partial^2 \phi}{\partial u^2} \right|_{jk} = \mu_+ \phi_{j,k+1} - (\mu_+ + \mu_-) \phi_{jk} + \mu_- \phi_{j,k-1} \tag{63b}$$

$$\left. \frac{\partial^2 \phi}{\partial x^2} \right|_{jk} = \lambda_+ \phi_{j+1,k} - (\lambda_+ + \lambda_-) \phi_{jk} + \lambda_- \phi_{j-1,k} \tag{63c}$$

$$\begin{aligned}
\left. \frac{\partial}{\partial x} \gamma \frac{\partial \phi}{\partial x} \right|_{jk} &= \frac{2}{\delta_+ + \delta_-} \left[ \gamma_{k+} \frac{\phi_{j+1,k} - \phi_{jk}}{\delta_+} - \gamma_{k-} \frac{\phi_{jk} - \phi_{j-1,k}}{\delta_-} \right] \\
&= \lambda_+ \gamma_{k+} \phi_{j+1,k} - (\lambda_+ \gamma_{k+} + \lambda_- \gamma_{k-}) \phi_{jk} + \lambda_- \gamma_{k-} \phi_{j-1,k}
\end{aligned} \tag{63d}$$

$\gamma_{k+}$  and  $\gamma_{k-}$  are respectively the values of  $\gamma$  at lethargy  $k$  in the right- and left-hand intervals.

The  $\eta$ 's,  $\mu$ 's and  $\lambda$ 's are functions of  $j$  and  $k$ , though we omit the indices for convenience. Our equations become

$$\sum_{p=-1}^1 \sum_{q=-1}^1 a_{pq} \phi_{j+p, k+q} = S_{jk}, \quad (64)$$

where  $S_{jk}$  is a source term, if any. Here the SPM differential equation can be written

$$\begin{aligned} -\alpha^0 \phi - \frac{\partial}{\partial u} \alpha^1 \phi + \frac{\partial^2}{\partial u^2} \alpha^2 \phi + \frac{\partial}{\partial x} \gamma^3 \frac{\partial}{\partial x} \alpha^3 \phi - \frac{\partial}{\partial x} \gamma^3 \frac{\partial}{\partial x} \gamma^4 \frac{\partial}{\partial u} \alpha^4 \phi - \\ - \frac{\partial}{\partial x} \gamma^3 \frac{\partial}{\partial u} \gamma^5 \frac{\partial}{\partial x} \alpha^3 \phi = S, \end{aligned} \quad (65)$$

where

$$\alpha^0 = \sigma - \sigma_s \quad (66a)$$

$$\alpha^1 = C_{10} \sigma_s \quad (66b)$$

$$\alpha^2 = \frac{1}{2} C_{20} \sigma_s \quad (66c)$$

$$\alpha^3 = \frac{1}{\sigma} C_{02} \sigma_s \quad (66d)$$

$$\alpha^4 = C_{12} \sigma_s \quad (66e)$$

$$\gamma^3 = \frac{1}{\sigma(1-v_0)} \quad (66f)$$

$$\gamma^4 = \frac{1}{\sigma} \quad (66g)$$

$$\gamma^5 = \frac{v_1}{1-v_0} \quad (66h)$$

The  $\alpha$ 's and  $\gamma$ 's are constant within each region. The  $a_{pq}$  that appear in eq. (71) are determined as follows:

$$\begin{aligned}
a_{\pm 1, -1} &= -\eta_{\pm} \lambda_{\pm} \gamma_{k\pm}^3 (\gamma_{k\pm}^4 \alpha_{k-1, \pm}^4 + \gamma_{k-1, \pm}^5 \alpha_{k-1, \pm}^3) \\
a_{\pm 1, 1} &= -\eta_{\pm} \lambda_{\pm} \gamma_{k\pm}^3 (\gamma_{k\pm}^4 \alpha_{k+1, \pm}^4 + \gamma_{k+1, \pm}^5 \alpha_{k+1, \pm}^3) \\
a_{0\pm 1} &= -\eta_{\pm} \alpha_{k\pm 1}^1 + \mu_{\pm} \alpha_{k\pm 1}^2 - a_{-1, \pm 1} - a_{1, \pm 1} \\
a_{\pm 1, 0} &= \lambda_{\pm} \gamma_{k\pm}^3 \left[ \alpha_{k\pm}^3 + (\eta_{+} + \eta_{-}) (\gamma_{k\pm}^4 \alpha_{k\pm}^4 + \gamma_{\pm}^5 \alpha_{k\pm}^3) \right] \\
a_{0, 0} &= -\alpha_k^0 + (\eta_{+} + \eta_{-}) \alpha_k^1 - (\mu_{+} + \mu_{-}) \alpha_k^2 - a_{-1, 0} - a_{1, 0}
\end{aligned} \tag{67}$$

If we are not at a boundary point and if the spatial integration mesh is constant in each region, then

$$a_{1, q} = a_{-1, q} \tag{68}$$

To solve eq. (64) we use a line relaxation method. The solution goes as follows: Suppose we want  $\phi_{jk}$ ,  $0 \leq j \leq J$ ,  $0 \leq k \leq K$ . An initial guess  $\phi_{jk}^{(0)}$  is made for  $\phi_{jk}$  at all interior mesh points, i.e., for  $1 \leq j \leq J-1$ ,  $1 \leq k \leq K-1$ . The conditions that the flux vanish at the boundary are given by the expressions

$$\phi_{jK} = 0, \quad 0 \leq j \leq J \tag{69a}$$

$$\phi_{0k} = 0, \quad 1 \leq k \leq K \tag{69b}$$

$$\phi_{Jk} = 0, \quad 1 \leq k \leq k. \tag{69c}$$

$\phi_{j0}$  is prescribed.



Given an estimate of the flux for lethargies (k-1) and (k+1), we can get a new estimate for lethargy k by the relation (64).

Then in the line relaxation procedure we get from eq. (64)

$$\sum_{p=-1}^1 a_{po}^{jk} \phi_{j+p,k}^{(i)} = g_{jk}^{(i)}, \quad (70)$$

where

$$g_{jk}^{(i)} = S_{jk} - \sum_{p=-1}^1 a_{p,-1}^{jk} \phi_{j+p,k-1}^{(i)} - \sum_{p=-1}^1 a_{p,i}^{jk} \phi_{j+p,k+1}^{(i-1)} \quad (71)$$

We have put indices j,k on the a-coefficients for explicitness. A superscript (i) represents the i<sup>th</sup> estimate of the flux. We start with k=1.  $\phi_{j+p,k-1}^{(i)}$  is then just the prescribed flux at u = 0. For k=2,  $\phi_{j+p,2}^{(0)}$  is the initial estimate. Thus  $g_{j1}^{(i)}$  can be determined from eq. (71). Solving eq. (70) then gives  $\phi_{j1}^{(i)}$ . The procedure is then repeated with k=2, etc., down to k = K-1. We now have  $\phi_{jk}^{(i)}$  everywhere. The process can clearly be iterated to give successively higher approximations. It can be shown that if the process converges, it converges to the correct answer.

The relaxation procedure could as easily have been carried out along lines of constant x. The equations that then replace (70) and (71) are

$$\sum_{q=-1}^1 a_{oq}^{jk} \phi_{j,k+q}^{(i)} = f_{jk}^{(i)} \quad (72)$$

$$f_{jk}^{(i)} = S_{jk} - \sum_{q=-1}^1 a_{1,q}^{jk} \phi_{j+1,k+q}^{(i-1)} - \sum_{q=-1}^1 a_{-1,q}^{jk} \phi_{j-1,k+q}^{(i)} \quad (73)$$

We use row iteration, although a column iteration or alternate row and column iteration are other possible procedures. Eqs. (70) and (72) are of the form,

$$a_n \psi_{n-1} + b_n \psi_n + c_n \psi_{n+1} = Q_n, \quad 0 < n < N. \quad (74)$$

Eq. (74) is solved by use of two auxiliary parameters  $Z_n$  and  $P_n$  which are defined recursively as

$$Z_n = - \frac{c_n}{b_n + a_n Z_{n-1}} \quad (75)$$

$$P_n = \frac{Q_n - a_n P_{n-1}}{b_n + a_n Z_{n-1}} \quad (76)$$

with

$$Z_0 = P_0 = 0. \quad (77)$$

Then

$$\phi_n = P_n + Z_n \phi_{n+1}. \quad (78)$$

Thus we have  $P_0, Z_0$ . Given  $P_{n-1}, Z_{n-1}$ , we can compute  $P_n, Z_n$  by eqs. (75) and (76) out to  $n = N-1$ .  $\phi_N$  is known. Given  $\phi_{n+1}$ , we can compute  $\phi_n$  by eq. (78), back to  $n=1$ . Thus the complete solution is given.

In a spatially symmetric situation, we take  $J = 0$  along the plane of symmetry, with  $-J \leq j \leq J$ . Symmetry implies that  $\phi_{1,k} = \phi_{-1,k}$  and that  $a_{1,q} = a_{-1,q}$ . For relaxation along lines of constant lethargy, we have to solve equations of the form (74) for  $0 < n \leq N$  with the added relation

$$a_0 \psi_{-1} + b_0 \psi_0 + c_0 \psi_1 = Q_0. \quad (79)$$

But because of the symmetry,  $a_0 = c_0$  and  $\psi_{-1} = \psi_1$ . Thus

$$\psi_0 = \frac{Q_0}{b_0} - \frac{2a_0}{b_0} \psi_1. \quad (80)$$

Comparison with eq. (78) gives

$$p_0 = \frac{Q_0}{b_0} \quad (81)$$

$$z_0 = \frac{2a_0}{b_0} \quad (82)$$

$\psi_n$  can then be found from eqs. (75), (76), and (78) for  $0 \leq n < N$ .

Relaxation along lines of constant  $x$  can be carried out either from  $N$  to  $0$  from  $0$  to  $N$ . However, for  $j = 0$ , eq. (23) becomes

$$f_{0k} = s_{0k} - \sum_{q=-1}^1 a_{1q}^{ok} \phi_{1,k+q}. \quad (83)$$

The  $i^{\text{th}}$  estimate for  $\phi_{1,k+q}$  is used in proceeding from  $K$  to  $0$ . The  $(i-1)^{\text{st}}$  estimate is perforce used if we proceed from  $0$  to  $K$ .

## F. Source Conditions

Assume we have a plane isotropic source  $\delta(x)\delta(u)$  at  $u = 0$ . For a uniform medium the slowing down density at  $u = 0$  can then be written

$$q(x) = \frac{1}{2} \sigma E_1(\sigma|x|), \quad (84)$$

since everything that scatters slows down at the collision point.  $\sigma$  is the cross section at  $u = 0$ . If there is little absorption near the source energy,  $q(x)$  is nearly constant except near  $x = 0$ . But except immediately around  $u = 0$ , we have

$$q = \xi \phi, \quad (85)$$

where  $\xi$  is the mean lethargy increase per collision.

Thus the flux is given correctly several  $\xi$ -units and more from the boundary if we take

$$\phi(x, 0) = \frac{1}{2\xi} E_1(\sigma|x|). \quad (86)$$

We use this as a boundary condition. It must be stressed that  $\phi(x, 0)$  is not a valid approximation to the flux very close to  $u = 0$ . It is the condition that must be used with the SPM equation to give the flux correctly away from  $u = 0$ . With this normalization both SPM and age theory reduce to the same asymptotic result for large  $u$ , as they should.

At an interface  $x_0$  we get the condition by assuming that the number of neutrons slowed down per unit time from  $u=0$  between  $x_0 - \epsilon\delta_-$  and  $x_0 + \epsilon\delta_+$  is given correctly by assuming that the flux at  $u = 0$

is continuous and linear in the intervals  $(x_0 - \epsilon \delta_-, x_0)$  and  $(x_0, x_0 + \epsilon \delta_+)$ .  $\delta_+$  and  $\delta_-$  are the distances from  $x_0$  to the next mesh points to the right and left, respectively. The natural requirement would be to let  $\epsilon = 1$ , but in order to get an expression which reduces to the correct one when the media on the two sides of the interface are identical, we let  $\epsilon$  approach zero. The precise condition at a single point is not especially critical, in any case. Thus we write for the slowing down density

$$\begin{aligned} q(x) &= \frac{\sigma_+}{2} E_1(|s + \sigma_+ (x - x_0)|) , & x_0 < x < x_0 + \epsilon \delta_+ \\ &= \frac{\sigma_-}{2} E_1(|s - \sigma_- (x_0 - x)|) , & x_0 - \epsilon \delta_- < x < x_0 , \end{aligned} \quad (87)$$

where

- $\sigma_+$  = total macroscopic cross section in interval  $x_0 < x < x_0 + \epsilon \delta_+$
- $\sigma_-$  = total macroscopic cross section in interval  $x_0 - \epsilon \delta_- < x < x_0$
- $s$  = total number of mean free paths between the origin and  $x_0$

We assume also that

$$\begin{aligned} q(x) &= \xi_+ \sigma_+ \phi(x) , & x_0 < x < x_0 + \epsilon \delta_+ \\ &= \xi_- \sigma_- \phi(x) , & x_0 - \epsilon \delta_- < x < x_0 \end{aligned} \quad (88)$$

Here

- $\xi_+$  = mean lethargy increase per collision in interval  $x_0 < x < x_0 + \epsilon \delta_+$
- $\xi_-$  = mean lethargy increase per collision in interval  $x_0 - \epsilon \delta_- < x < x_0$

Then

$$\begin{aligned} \int_{x_0 - \epsilon \delta_-}^{x_0 + \epsilon \delta_+} q(x) dx &= \int_{x_0 - \epsilon \delta_-}^{x_0} \frac{\sigma_-}{2} E_1(|s - \sigma_-(x_0 - x)|) dx + \int_{x_0}^{x_0 + \epsilon \delta_+} \frac{\sigma_+}{2} E_1(|s + \sigma_+(x - x_0)|) dx \\ &= \frac{1}{2} \int_{s - \epsilon \sigma_- \delta_-}^{s + \epsilon \sigma_+ \delta_+} E_1(|y|) dy. \end{aligned} \quad (88)$$

Also

$$\int_{x_0 - \epsilon \delta_-}^{x_0 + \epsilon \delta_+} q(x) dx = \xi_- \sigma_- \int_{x_0 - \epsilon \delta_-}^{x_0} \phi(x) dx + \xi_+ \sigma_+ \int_{x_0}^{x_0 + \epsilon \delta_+} \phi(x) dx. \quad (90)$$

Now in the limit  $\epsilon \rightarrow 0$ , we get by equating expressions (89) and (90)

$$\frac{1}{2} E_1(s) (\epsilon \sigma_+ \delta_+ + \epsilon \sigma_- \delta_-) = \phi(x_0) (\epsilon \xi_+ \sigma_+ \delta_+ + \epsilon \xi_- \sigma_- \delta_-),$$

or finally

$$\phi(x_0) = \frac{1}{2} E_1(s) \frac{\sigma_+ \delta_+ + \sigma_- \delta_-}{\xi_+ \sigma_+ \delta_+ + \xi_- \sigma_- \delta_-}. \quad (91)$$

For an interior point, this reduces to

$$\phi(x_0) = \frac{1}{2} E_1(s), \quad (92)$$

as expected.

The  $E_1$  source gives a problem in a numerical calculation because it is singular at the origin. The criterion we use to avoid the singularity is that the total number of neutrons slowed down per unit time from  $u = 0$  in the interval  $-\delta_- < x < \delta_+$  is given by a

three-point formula in terms of the continuous and piecewise linear flux  $\phi(x)$  at  $u = 0$ .

Thus eqs. (87) and (88) hold, with  $x_0 = 0$ ,  $s = 0$ ,  $\epsilon = 1$ .

$$\begin{aligned}
 \int_{-\delta_-}^{\delta_+} q(x) dx &= \int_{-\delta_-}^0 \frac{\sigma_-}{2} E_1(|\sigma_- x|) dx + \int_0^{\delta_+} \frac{\sigma_+}{2} E_1(\sigma_+ x) dx \\
 &= \frac{1}{2} \int_0^{\sigma_- \delta_-} E_1(y) dy + \frac{1}{2} \int_0^{\sigma_+ \delta_+} E_1(y) dy = \frac{1 - E_2(\sigma_- \delta_-)}{2} + \frac{1 - E_2(\sigma_+ \delta_+)}{2} \\
 &= \frac{1}{2} \left[ 2 - e^{-\sigma_- \delta_-} + \sigma_- \delta_- E_1(\sigma_- \delta_-) - e^{-\sigma_+ \delta_+} + \sigma_+ \delta_+ E_1(\sigma_+ \delta_+) \right] \quad (93)
 \end{aligned}$$

We have used the relations

$$\int_p^\infty E_1(y) dy = E_2(p) \quad (94)$$

$$E_2(0) = 1 \quad (95)$$

$$E_2(p) = e^{-p} - p E_1(p) \quad (96)$$

Also,

$$\begin{aligned}
 \int_{-\delta_-}^{\delta_+} q(x) dx &= \int_{-\delta_-}^0 \xi_- \sigma_- \phi(x) dx + \int_0^{\delta_+} \xi_+ \sigma_+ \phi(x) dx \\
 &= \xi_- \sigma_- \frac{\delta_-}{2} [\phi(-\delta_-) + \phi(0)] + \xi_+ \sigma_+ \frac{\delta_+}{2} [\phi(0) + \phi(\delta_+)] \quad (97)
 \end{aligned}$$

Since by assumption,  $-\delta_-$  and  $\delta_+$  are not interface points,

$$\phi(\pm\delta_{\pm}) = \frac{1}{\sigma_{\pm} \xi_{\pm}} q(\pm\delta_{\pm}) = \frac{1}{2\xi_{\pm}} E_1(\sigma_{\pm}\delta_{\pm}) \quad , \quad (98)$$

and so equating the right-hand sides of eqs. (93) and (97) and using (98), we have

$$\begin{aligned} \frac{1}{2} \left[ 2 - e^{-\sigma_- \delta_-} + \sigma_- \delta_- E_1(\sigma_- \delta_-) - e^{-\sigma_+ \delta_+} + \sigma_+ \delta_+ E_1(\sigma_+ \delta_+) \right] = \\ = \frac{1}{2} (\xi_- \sigma_- \delta_- + \xi_+ \delta_+) \phi(0) + \frac{1}{4} \sigma_- \delta_- E_1(\sigma_- \delta_-) + \frac{1}{4} \sigma_+ \delta_+ E_1(\sigma_+ \delta_+) \end{aligned}$$

or finally,

$$\phi(0) = \frac{2 - e^{-\sigma_- \delta_-} + \frac{1}{2} \sigma_- \delta_- E_1(\sigma_- \delta_-) - e^{-\sigma_+ \delta_+} + \frac{1}{2} \sigma_+ \delta_+ E_1(\sigma_+ \delta_+)}{\xi_- \sigma_- \delta_- + \xi_+ \sigma_+ \delta_+} \quad (99)$$

Eq. (99) gives the value we use for  $u = 0$  at the origin.



### G. Boundary Conditions

Since we are working with an equation essentially of the elliptic type, we specify one boundary condition all around the boundary. The computations use a rectangular region ( $a < x < b$ ,  $0 < u < u_c$ ). The source condition at  $u=0$  has been discussed. We use the condition  $\phi(x, u_c) = 0$  at the cutoff lethargy  $u_c$ . It was shown in the previous summary report<sup>1</sup> that the precise condition at  $u_c$  does not affect the solution except in the immediate vicinity of  $u_c$ , if the condition is at all a reasonable one. The present spatial boundary conditions are that the flux vanishes at  $a$  and  $b$ . One could use instead derivative boundary conditions, i.e., that  $\frac{\partial \phi}{\partial x}$  is equal to some constant on the boundaries. This is, in fact, the condition on the line of symmetry for the symmetrical case, where  $\frac{\partial \phi}{\partial x} = 0$ .

### H. Inelastic Scattering

Inelastic scattering must be treated as an absorption followed by a reemission at a lower energy, as in multigroup theory. It presents two problems, one intrinsic and one purely practical. The practical problem is that of time and memory requirements in the machine computation. We get an effective source of strength

$$S(x, u) = \int \sigma(x; u', u) \phi(x, u') du' , \quad (100)$$

where

$\sigma(x; u', u)$  = inelastic macroscopic scattering cross section at  $x$   
for neutron of lethargy  $u'$  to scatter to  $u$ , per unit  
lethargy range about  $u$ .

$S$  is treated as an inhomogeneous neutron source. The appropriate term in the SPM equation is  $\psi_0$ , the first collision density of neutrons whose source strength is given by  $S$ .

$$\psi_0(x, u) = \frac{1}{2} \sigma(u) \int E_1(|s|) S(x', u) dx', \quad (101)$$

where

$$s = \int_{x'}^x \sigma(u, x'') dx''.$$

Just as in multigroup diffusion calculations, however, we will not take account of the transport of these neutrons between the point of inelastic scattering and the point at which they next collide. That is, we take

$$\psi_0(x, u) = S(x, u). \quad (102)$$

This approximation eases the very considerable computation that would be required to use eq. (101).

The intrinsic problem with inelastic scattering lies in the fact that any source in the interior of the  $u$ -interval, i.e., for  $u > 0$ , can propagate in both directions in lethargy. While the propagation to lower lethargies is damped fairly rapidly with decreasing  $u$ , this part of the contribution is certainly unphysical. Further, the flux is not correct even above this interior source lethargy until about an interval  $\Delta u \approx \xi$  away. It is certainly true, however, that if the flux inelastically scattered to an interval whose width is of the order of  $\xi$  is small compared to that slowed down by elastic scattering, the error is small. That is, in that interval the error is small by

hypothesis, and in any case does not propagate very far. The latter property implies that the error is not cumulative, but only local so that it is limited in magnitude everywhere.

It should be remarked that these difficulties are present in part in ordinary multigroup theory whenever the relation  $q = \xi \sigma \phi$  is used to connect the slowing down density and the flux.

The code takes inelastic cross sections in two forms: either as the cross section  $\sigma_{in}(u', E)$  at  $u'$  per unit final energy about  $E$ , tabulated as a function of  $u'$  and  $E$ , or as an excitation cross section  $f_{in}(u', Q_i)$  tabulated as a function of  $u'$  and the excitation energy  $Q_i$ . In the available tabulated inelastic cross section data  $f_{in}(u', Q_i)$  may be available as interpolated in the initial lethargy directly from experiment, for the lowest excitation levels  $Q_i$ . At higher incident energies one resorts to calculated cross sections in the form  $\sigma_{in}(u', E)$ .

In general,  $f_{in}(u', Q_i)$  may not sum precisely to the total observed inelastic cross section at  $u'$  because of experimental inaccuracies. We therefore define the normalized excitation cross section

$$g_i(u) = f_{in}(u, Q_i) \frac{\sigma_{in}(u)}{\sum_l f_{in}(u, Q_l)} \quad (103)$$

$g_i$  has the required property that

$$\sum_i g_i(u) = \sigma_{in}(u). \quad (104)$$

$\sigma_{in}(u)$  is the cross section for neutron production by inelastic scattering. In terms of the  $(n, n')$  and  $(2, 2n)$  cross sections it is

$$\sigma_{in}(u) = \sigma_{n, n'}(u) + \sigma_{n, 2n}(u). \quad (105)$$

Since  $\sigma_{in}(u', E)$  is computed while  $\sigma_{in}(u)$  is measured, integration of  $\sigma_{in}(u, E)$  over  $E$  will not in general give  $\sigma_{in}(u)$ . Again we must impose a normalization. In the code, it is assumed that  $\sigma_{in}(u', E)$  is linear in  $E$  between each successive tabulated values. It is further assumed that if  $E$  takes on the values  $E_i$  and if there are  $P$  values of  $i$  in the tabulation, that

$$\begin{aligned} E_{P+1} &= 0 \\ \sigma_{in}(u', 0) &= 0 \\ E_{i+1} &< E_i \\ \sigma_{in}(u', E) &= 0, \quad E > E_1. \end{aligned}$$

Then we can get a normalized cross section

$$\sigma_{in}'(u', E) = \sigma_{in}(u', E) \frac{\sigma_{in}(u')}{\frac{1}{2} \sum_{i=1}^P \left\{ \sigma_{in}(u', E_i) + \sigma_{in}(u', E_{i+1}) \right\} (E_i - E_{i+1})} \quad (106)$$

In terms of  $g_i$  and  $\sigma_{in}'$ , the differential inelastic neutron cross section is

$$\begin{aligned} \sigma(u', u) &= E \sigma_{in}(u', E), \quad u' < u_{k_1} \\ &= \sum_i g_i(u') \delta(E' - E - Q_i) E, \quad u' \geq u_{k_1}^* \end{aligned} \quad (107)$$

Here  $u_{k_1}$  is the smallest lethargy at which  $f_{in}(u, Q_i)$  is given. For

$u_{k_2} < u' < u_{k_1}$ , where  $u_{k_2}$  is the largest lethargy for which we use the  $\sigma_{in}(u', E)$  data, the codes takes

$$\sigma_{in}'(u', E) = \sigma_{in}'(u_{k_2}, E). \quad (108)$$

---

\*Eq. (107) assumes that the excitation energy  $Q_i$  equals the neutron energy loss in the c.m. system. While not strictly true, this is an adequate approximation for our purposes.

Elsewhere we interpolate linearly in  $u'$ , for both  $\sigma'_{in}(u', E)$  and  $g_i(u')$ .

In eq. (107),

$$E' = E_0 e^{-u'} \quad (107)$$

Note that

$$Q_i < E_0 e^{-u} \quad (110)$$

Substituting eq. (107) in eq. (100) and using eq. (107), we have, dropping the spatial variable  $x$ ,

$$\begin{aligned} S(u) &= \int_0^u \sigma(u', u) \phi(u') du' \\ &= \int_0^u \sigma(u', E) E \phi(u') du', \quad u < u_{k1} \\ &= \int_0^{u_{k1}} \sigma'_{in}(u', E) E \phi(u') du' + \sum_i E \int_{u_{k1}}^u g_i(u') \delta(E' - E - Q_i) \phi(u') du', \\ &\quad u > u_{k1} \quad (111) \end{aligned}$$

In our mesh scheme, the lethargy takes on the value  $u_k$ , and integration is by the trapezoidal rule. Let us define

$$G_k = \frac{E_k}{2} \sum_{i=1}^{k_0-1} \left\{ \phi(u_i) \sigma'_{in}(u_i, E_k) + \phi(u_{i+1}) \sigma'_{in}(u_{i+1}, E_k) \right\} (u_{i+1} - u_i), \quad (112)$$

with

$$\begin{aligned} k_0 &= k, & u_k &< u_{k1} \\ &= k_1, & u_k &\geq u_{k1} \end{aligned} \quad (113)$$

$E_k$  and  $u_k$  are related by the standard expression

$$E_k = E_0 e^{-u_k} \quad (109a)$$

Then

$$\int_0^{u_{k_0}} \sigma_{in}(u', E) E \phi(u') du' = G_{k_0}. \quad (114)$$

Also,

$$\begin{aligned} E \int_u^{u_k} g_i(u') \delta(E' - E_k - Q_i) \phi(u') du' &= \\ &= \int_{E_k}^{E_{k_1}} g_i\left(\ln \frac{E_0}{E'}\right) \phi\left(\ln \frac{E_0}{E'}\right) \delta(E' - E_k - Q_i) \frac{E_k}{E'} dE' \\ &= g_i\left(\ln \frac{E_0}{E_k + Q_i}\right) \phi\left(\ln \frac{E_0}{E_k + Q_i}\right) \frac{E_k}{E_k + Q_i} H(E_{k_1} - E_k - Q_i) \end{aligned} \quad (115)$$

$H$  is again the step function defined previously:

$$\begin{aligned} H(\xi) &= 1, & \xi > 0 \\ &= 0, & \xi < 0. \end{aligned} \quad (3)$$

Let

$$\alpha_{ik} = \frac{E_k + Q_i}{E_k} = 1 + \frac{Q_i}{E_0} e^{u_k} \quad (116)$$

and

$$v_{ik} = \ln \alpha_{ik}. \quad (117)$$

Then

$$\ln \frac{E_0}{E_k + Q_i} = \ln \frac{E_0}{E_k} + \ln \frac{E_k}{E_k + Q_i} = u_k - v_{ik}. \quad (118)$$

Substituting eqs. (114) and (115) in eq. (111) and using eqs. (116) and (118), we get finally

$$S(u_k) = G_{k_0} + \sum_i g_i (u_k - v_{ik}) \theta(u_k - v_{ik}) H(E_{k_1} - E_k - Q_i). \quad (119)$$

Eqs. (113), (109a), (3), (116), and (117) define all the parameters.

Eq. (119) holds at every spatial mesh point  $j$  in the inelastic scattering medium.

To determine what value of  $S(u_k)$  to use at a boundary point of an inelastic scattering medium, let us consider a situation where there is one inelastic scattering medium to the right of spatial mesh point  $j$  and another to the left. Then we assume that the total source of inelastically scattered neutrons is represented as being continuous at  $x_j$  and linear between  $x_{j-1}$  and  $x_j$  and between  $x_j$  and  $x_{j+1}$ . Thus

$$\int_{x_{j-1}}^{x_{j+1}} S(x, u_k) dx = \frac{\delta_-}{2} [S_{j-1,k} + S_{jk}] + \frac{\delta_+}{2} [S_{jk} + S_{j+1,k}] = S(u_{k+}) \delta_+ + S(u_{k-}) \delta_- \quad (120)$$

Here

$$S_{jk} = S(x_j, u_k). \quad (121)$$

and

$$S_{j+1,k} = S(u_{k+}). \quad (122)$$

Then

$$S_{jk} = \frac{\delta_+ S(u_{k+}) + \delta_- S(u_{k-})}{\delta_+ + \delta_-} \quad (123)$$

In the spirit of the derivation of the flux at an interface for  $u=0$ , eq.(123) should hold not for the density  $S$  of inelastically scattered neutrons, but for the cross sections  $\sigma'_{in}(u,E)$  and  $g_i(u)$ . However, prescription (123) is much simpler. In addition, the overall error is small, probably much smaller than the error involved in the assumption (102).



### III. Results

#### A. Carbon

Comparisons were made of SPM results with those of age theory and of a method due to Kaper.<sup>2</sup> The medium was carbon with an assumed constant cross section. There is no absorption.

The flux given by age theory can be written

$$\phi(x, u) = \frac{1}{\sigma \xi} e^{\frac{-x^2}{4\tau}} \sqrt{\frac{4\pi\tau}{\sigma \xi}}$$

Here the geometry is that of an infinite plane source of strength

$$S(x, u) = \delta(x) \delta(u)$$

with no first flight correction.

$\tau$  is the neutron age, given by

$$\tau = \frac{u}{3\sigma^2 \xi}$$

The age theory solution is tabulated in Table I.

Kaper<sup>2</sup> has developed a treatment which is essentially a consistent expansion in powers of  $1/A$ , valid also for variable cross sections. Since one can look on the SPM as an expansion in powers of  $1/A$ , though not a consistent one (since it gives certain higher order terms), it is of interest to compare the two methods. Kaper has given results for the first order solution; i.e., that good to linear terms in  $1/A$ . The SPM equation contains in addition the terms in  $1/A^2$  and certain, but not all, higher terms. For carbon ( $A = 12$ ), the differences should not be great.

For the comparison we use Kaper's solution including first flight, that is, with a first flight correction, normalized to the age theory results at  $\Sigma x = 1$ ,  $u = 15$ . Of the points given by Kaper, this is the one for which age theory should be best (small  $x$ , large  $u$ ), and so the results were normalized accordingly. This solution is shown in Table II.

We have two sets of SPM results for this problem. Both used an  $E_1$  source. One, given in Table III, is the solution of the third-order equation. The other, shown in Table IV, is the solution when the third-order terms (i.e.,  $\gamma_4$  and  $\gamma_5$ ) are assumed zero. Note that the effect of the third-order terms in this problem is negligible.

In comparing the solutions given in Tables I-III, we note that agreement is very close at smaller distances, but for larger values of  $x$ , the SPM solution is flatter - smaller for large  $u$  and much larger for small  $u$  - than either the age or Kaper's solution. Certainly the increase for small  $u$  is an improvement. The differences for large  $u$  are not great and it is not clear whether or not they are significant.

TABLE I. DIFFUSION THEORY (A = 12)

$$\phi = \frac{1}{4} \sqrt{\frac{6A}{\pi u}} e^{-\frac{(\Sigma x)^2}{2Au}}$$

$\begin{array}{c} \Sigma x \\ u \end{array}$	1	2	5	8	10
1	1.06	0.726	0.053	-	-
3	0.663	0.585	0.244	0.048	0.010
5	0.522	0.484	0.286	0.108	0.044
8	0.417	0.398	0.286	0.156	0.089
10	0.374	0.360	0.277	0.170	0.108
12	0.342	0.331	0.266	0.177	0.122
15	0.306	0.299	0.251	0.181	0.134

TABLE II. KAPER'S APPROXIMATION<sup>2</sup> FOR FLUX (A = 12)

$\Sigma x$ u	1	2	5	8	10
1	1.01	0.661	0.073	-	-
2	0.639	0.569	0.227	0.048	0.010
3	0.507	0.479	0.271	0.108	0.037
8	0.410	0.388	0.276	0.154	0.078
10	0.364	0.350	0.264	0.168	0.098
12	0.335	0.324	0.258	0.176	0.108
15	0.306	0.287	0.236	0.181	0.128

TABLE III. SPM FLUX ( $A = 12$ ) - WITH THIRD ORDER TERMS

$\Sigma x$ $u$	1	2	5	8	10
1	1.07	0.760	0.098	-	-
3	0.676	0.605	0.280	0.070	0.020
5	0.534	0.499	0.313	0.131	0.053
8	0.426	0.408	0.302	0.165	0.079
10	0.381	0.368	0.286	0.167	0.083
12	0.347	0.336	0.267	0.162	0.082
15	0.305	0.296	0.240	0.149	0.076

TABLE IV. SPM FLUX ( $A = 12$ ) - WITHOUT THIRD ORDER TERMS

$\begin{array}{c} \Sigma x \\ u \end{array}$	1	2	5	8	10
1	1.09	0.728	0.096	-	-
3	0.691	0.611	0.270	0.069	0.020
5	0.541	0.504	0.309	0.127	0.051
8	0.430	0.411	0.301	0.162	0.077
10	0.384	0.370	0.285	0.165	0.082
12	0.347	0.337	0.267	0.161	0.081
15	0.306	0.297	0.241	0.149	0.076

## B. Hydrogen

A number of problems were run for hydrogen, since the ability to treat hydrogen was considered a major part of the program. Some used an 18-Mev source and some an 8-Mev source, with x- and u-meshes of various sizes. Results for 8-Mev sources are not yet available. All of the 18-Mev problems failed. The reason is important and instructive.

All of the 18-Mev problems included the third order terms. Basically, they failed because  $a_{1,-1}$  and  $a_{-1,-1}$  (eq. 67) were too large.  $a_{10}$  could therefore be small and even negative. If we were dealing with a delta function source, for instance, i.e., a source of unity at  $(j,k) = (0,0)$ , where  $j$  and  $k$  are respectively the x and u-indices, this would imply that  $\phi(1,0) < 0$ . This is obviously inadmissible. The situation with the  $E_1$  source was somewhat more complicated, but fundamentally the same. Not only were some fluxes negative, but the error propagated from iteration to iteration and the iteration procedure rapidly diverged. It should be remarked that  $a_{1,-1}$  and  $a_{-1,-1}$  can become too large only in the case of variable cross sections.

The conclusion from all this is that if the cross section variation is too great, trouble can be expected from the third-order terms. This bears on the problem of treating resonances. If we had hoped to improve on the second order equation by adding third-order terms, one must be extremely careful with variable cross sections. We have not been able to deduce any real rules for predicting when the third-order terms help.

### C. Modification of Diffusion Theory Current by SPM

To see how the additional terms in the SPM equation modify the diffusion theory expression for the current, we have two procedures. In one, we can assume that the change from age-diffusion theory is a small perturbation and apply the derivatives in the additional terms to the age-theory solution. In the other, we look at the ratio of the additional terms in the difference expression for the current to the diffusion term for one of our numerical solutions. We will consider both methods, for a medium with constant cross section and no absorption.

The age-diffusion solution is

$$\phi = \frac{1}{\sigma \xi} \frac{e^{-\frac{x^2}{4\tau}}}{\sqrt{4\pi\tau}},$$

with

$$\tau = \frac{u}{3\sigma^2 \xi}$$

The SPM expression for the current in a constant cross section medium is

$$J = \gamma_3 \left[ \alpha_{32k} \frac{\partial \phi}{\partial x} - (\gamma_4 \alpha_4 + \gamma_5 \alpha_3) \frac{\partial^2 \phi}{\partial x \partial u} \right]$$

We are then interested in R, the ratio of the additional term in this expression to the diffusion term.

$$R = \frac{\gamma_4 \alpha_u + \gamma_5 \alpha_3}{\alpha_3} \frac{\partial^2 \phi}{\partial x \partial u} \left( \frac{\partial \phi}{\partial x} \right)^{-1}.$$



In our case

$$\frac{\gamma_4 \alpha_u + \gamma_5 \alpha_3}{\alpha_3} = \frac{v_1}{1-v_0} + \frac{C_{12}}{C_{02}} = \xi + \frac{v_1}{1-v_0}$$

for an isotropic flux.

We take derivatives of the unperturbed age theory solution

$$\ln \phi = \ln (\sigma \xi) - \frac{1}{2} \ln (4\pi) - \frac{1}{2} \ln \tau - \frac{x^2}{4\tau}$$

$$\frac{1}{\phi} \frac{\partial \phi}{\partial x} = - \frac{x}{2\tau}$$

$$\frac{1}{\phi} \frac{\partial \phi}{\partial \tau} = \left[ \frac{1}{2\tau} - \frac{x^2}{4\tau^2} \right]$$

$$\begin{aligned} \frac{\partial^2 \phi}{\partial x^2 \partial u} &= \frac{\partial}{\partial u} \left( \frac{x}{2\tau} \phi \right) = - \frac{1}{3\sigma^2 \xi} \frac{\partial}{\partial \tau} \left( \frac{x}{2\tau} \phi \right) \\ &= \frac{1}{3\sigma^2 \xi} \left( - \frac{x}{2\tau^2} \phi + \frac{x}{2\tau} \frac{\partial \phi}{\partial \tau} \right) \\ &= \frac{1}{3\sigma^2 \xi} \left( \frac{x}{2\tau^2} \phi + \frac{x}{2\tau} \left[ \frac{1}{2\tau} - \frac{x^2}{4\tau^2} \right] \right) \\ &= \frac{x}{12\sigma^2 \xi \tau^2} \left[ 3 - \frac{x^2}{2\tau} \right] \phi \end{aligned}$$

Thus the analytical approximation to R is

$$R_{an} = \left( \xi + \frac{v_1}{1-v_0} \right) \frac{3 - \frac{x^2}{2\tau}}{6\sigma^2 \xi \tau} = \left( \xi + \frac{v_1}{1-v_0} \right) \frac{3 \left[ 1 - \frac{\xi (6x)^2}{2u} \right]}{2u}$$

For carbon, in our problem,

$$\xi = 0.15779$$

$$\frac{v_1}{1-v_0} = \gamma_5 = 0.04953$$

$$\sigma = 1$$

Then

$$R_{an} = 0.10826 \frac{3 \left[ 1 - 0.078895 \frac{x^2}{u} \right]}{2u \cdot 43}$$

We compare this with the numerical approximation,  $R_{\text{num}}$ , in which the derivatives are evaluated by differences from our numerical results. The results are shown in Table V.

TABLE V. EFFECT OF HIGHER ORDER TERMS ON THE CURRENT

$x(\text{mfp})$	$u$	$R_{\text{anal}}$	$R_{\text{num}}$
2	1	0.111	0.108
2	2	0.0683	0.0667
2	5	0.0304	0.0299
2	10	0.0157	0.0098
5	5	0.0197	0.0194
5	10	0.0130	0.0075
10	5	-0.0188	-0.0201
10	10	0.0034	0.0022

We note that except near the origin and for small lethargies the SPM correction to the current is small - of the order of a few percent or less. Where  $R_{\text{anal}}$  and  $R_{\text{num}}$  differ appreciably, the correction is negligible.

#### IV. Operating Instructions - SPM Code

##### A. Changing Tape Designations

The 3 magnetic tapes required by the SPM code are assigned by a small subroutine called CHANTP. The copy of the SPM deck issued at the time of this report defines the problem input data tape to be logical tape number 2, the output tape to be logical tape number 3, and the tape which stores complete nuclide data for a series of nuclides to be logical tape number 5.

The tape designations may be inconsistent with the monitor system of a given 7090 installation. Therefore a simple process for making the necessary changes has been provided. The subroutine CHANTP is listed below.

##### SUBROUTINE CHANTP

(Common, dimension, and equivalence statements)

NUTAPE = 5

KTIN = 2

KTOUT = 3

RETURN

END (1,0,0,0,0,0,1,0,0,0,0,0,0,0,0)

##### Statements of CHANTP subroutine

KTIN defines the problem input tape, KTOUT indicates the output tape, and NUTAPE denotes the nuclide data tape. To redefine tapes for SPM:

1. Punch the proper logical tape number in the 3 statements which define KTIN, KTOUT, & NUTAPE,
2. Remove the old binary CHANTP program and
3. Recompile CHANTP (and possibly execute a SPM problem).

The use of the new binary CHANTP subroutine in the SPM binary deck or tape makes the code usable at the installation.

## B. Operation Instructions for a Problem Run

1. Since most 7090 installations will accept Fortran codes only when under monitor control, only one provision (see below) for console control of the SPM code has been made. It is generally necessary to provide the 7090 machine operator with only

- a. the SPM code in card deck or magnetic tape form,
- b. the input data, usually on cards, for the series of problems to be run,
- c. the nuclide data storage tape (NUTAPE) which generally will not be written on.

Sense Switch 6 must be up. In the usual case nothing further can be done by the user of the program.

### 2. Console Control of the SPM code

If sense switch 6 is depressed the code will stop after computing and outputting a complete array of fluxes. The iteration number of the flux computation loop will be printed both on-and-off line. This console operation should be used only when time considerations indicate that the problem being run should be terminated. Depressing sense switch 6 will allow the program user to obtain all information available concerning the last flux iteration at the time the problem was stopped. The program user may then alter the input of convergence conditions so that the further use of sense switch 6 will become unnecessary.

NOTE: In the following input table we use the following definitions:

$$d_1 = a_{-1,-1}$$

$$d_6 = a_{1,0}$$

$$d_2 = a_{0,-1}$$

$$d_7 = a_{-1,1}$$

$$d_3 = a_{-1,-1}$$

$$d_8 = a_{0,1}$$

$$d_4 = a_{-1,0}$$

$$d_9 = a_{1,1}$$

$$d_5 = a_{0,0}$$

$$d_{10} = S_{jk}$$

where the  $a_{pq}$  and  $S_{jk}$  are those in eq. (64).

The columns described refer to the 72 columns available on a standard IBM punched card.

# Input Data for SPM Code

Category No.	General Description	Format	Specific Input Quantity
1.	Titles and problem Identification Data	(12A6)	Date in columns (1-12) A problem identification number in columns (13-18) Any comment in columns (19-72) This data is printed in output and as page headings.
2.	Fixed point or integer input data:  Note that blank columns are treated as zeroes. Hence all integer data must occupy right hand columns of their fields	(24I3)	MXIFL, Maximum number of iterations before problem terminates itself. It is placed on the first card of category 2 Columns (1-13)  KLIMIT, Maximum number of lethargy levels included in convergence tests, Columns (4-6)  J2, the number of spatial points, including boundaries, Columns (7-9)  K2, the number of lethargy points, including boundaries, Columns (10-12)  IPCY, the number of iterations on the flux per printout of abbreviated convergence data (see output description). Columns (13-15)  IMALP, the number of flux iterations at which an indication of "Excessive Iterations" is printed out both on-line and off-line and beyond which all flux convergence data is

Category No.	General Description	Format	Specific Input Quantity
2.			printed out; the problem continues, however. Columns (16-18)
			<p>MKO, the mesh size of the lethargy output printout. Though the computation is carried out in its latest stages for all of the K2 lethargy points, output occurs for only those points <math>R=1, 1+MKO, \dots 1+nMKO, \dots K2</math>. Columns (19-21)</p>
			<p>MJO, the mesh size of spatial point output printout. Only the fluxes corresponding to <math>j=1, 1+MJO, \dots 1+nMJO, \dots J2</math> are printed out. Columns (22-24)</p>
			<p>IDEBUG, an indicator.</p> <p>If IDEBUG=20, there is no nuclide data storage tape. Option 5, category input then computes or obtains the necessary nuclide data. Columns (25-27)</p>
			<p>MMT, the number of entries in the mesh size table MTAB (see below). Columns (28-30)</p>
			<p>MTAB(I), <math>I=1, MMT</math>. A table of the mesh sizes to be used successive in the compute-flux-array computation. The table consists of pairs of mesh sizes for space pt. mesh, and lethargy pt. mesh, respectively. Coarse mesh pairs, monotonically decreasing, precede the finest mesh size pair (1,1) which are then followed by two zeroes. By far the most usual input for this</p>

Category No.	General Description	Format	Specific Input Quantity
2.			<p>table of MTAB, where MMT=4, is 1, 1, 0, 0. Next(MMT x 3 columns)</p> <hr/> <p>MIFLAG, the number of entries for the input table of flux arguments data (see table ALPLAY in category 3 input). Next three columns.</p> <hr/> <p>KBGIHS, the number of the lethargy point at which the arbitrary input of the D<sub>10</sub> (inhomogeneous source terms) begins. Next 3 columns.</p> <hr/> <p>KIST, the number of the last lethargy pt. at which there will be arbitrary input of the D<sub>10</sub> terms. All lethargy points from KBGIHS to KIST will have this input whenever KBGIHS ≠ 0. Next 3 columns.</p> <hr/> <p>INONU, the number of geometrically defined regions, each of constant nuclear composition. Next 3 columns.</p> <hr/> <p>ID 10 FS, If this indicator = 0, fission is treated as absorption. At this time the indicator must be zero. Next 3 columns.</p> <hr/> <p>ID 10 IE, If this indicator = 0, inelastic scattering is treated as absorption.  At this time this indicator must be zero. Next 3 columns.</p>

Category No.	General Description	Format	Specific Input Quantity
2.			<p>ISOUR<sup>1</sup>            If this indicator = 0, a table will be required in category 6 input. This table is the spatial source at the first lethargy level, <math>k=1</math>.            If this indicator &gt; 0 an <math>E_1</math> source (as described in the text) is computed with its origin at the spatial point <math>x = 0.0</math>.            Next 3 columns.</p> <hr/> <p>ID 10,            If this indicator = 0, there is no arbitrary input of <math>D_{10}</math> sources. If this indicator 0 an input table FIST, category 7, will load <math>D_{10}</math> sources directly from input for each lethargy level from KBGINS to KIST.            Next 3 columns.</p> <hr/> <p>IROCO.            If this indicator = 0, the computation of the flux array will proceed by row iterations only. If IROCO = 0, the flux computation will proceed alternately by row and column iterations.            Next 3 columns.</p> <hr/> <p>ISYMM            If this indicator = 1 the flux configuration will be computed symmetric about the left edge of the array (usually <math>x = 0</math>). This condition of symmetry applies only for IROCO = 0, i.e. row iteration only used in the computation of flux.            Next 3 columns.</p> <hr/>



Category No.	General Description	Format	Specific Input Quantity
3.	<p>Floating Point Input Data</p> <p>Each Single entry occupies 8 columns.</p> <p>Each input entry of the form <math>.fff \times 10^{+ee}</math> is expressed <math>(.fffE+ee)</math> in the 8 column field.</p> <p>(A certain economy is permitted by Fortran in preparing E format Floating Point input numbers.</p> <p>See ITM Reference Manual, 709/7090 FORTRAN PROGRAMMING SYSTEM p.45, bottom.)</p>	9E(8.2)	<p>ALPLAY (I), I = 1, MIFLAG.</p> <p>This table defines the spatial and lethargy coordinates, for the finest mesh, of the flux array. The space defining data is <math>x_1, \Delta x_1, x_2, \Delta x_2, \dots, x_{\text{INONU}}, \Delta x_{\text{INONU}}, x_{\text{INONU}+1}, 0.0.</math></p> <p><math>x_m</math> is the coordinate of the lefthand edge of the mth physical region; <math>\Delta x_m</math> is the constant interval within that region. Spatial data is terminated by a constant interval distance=0.0. The mesh point distances give the points for the finest spatial mesh: hence there are J2 such points. The table continues with the beginning entry of the lethargy coordinates (usually 0.0). Then follows the constant <math>\Delta u</math>, the maximum lethargy, and the indicator value 0.0. With 1 spatial region, therefore, there would be 8 entries or 64 columns to this table. Where INONU = no. of regions, use next 16 INONU + 48 columns.</p>
			<p>E,</p> <p>criterion for flux convergence. The maximum residual obtained from the comparison of each old flux to the newly computed flux must be less than this value for convergence to occur. Next 8 columns.</p>
			<p><math>E_1</math>.</p> <p><math>E_1</math> is a very small positive number. The number of flux values, whose absolute value in any given iteration is smaller than <math>E_1</math>, is counted and stored in NCON (location 53151g). Next 8 columns.</p>
			<p>ENZRI</p> <p>The energy at which lethargy <math>u = 0</math> for the particular problem. Next 8 columns.</p>

Category No.	General Description	Format	Specific Input Quantity
3.			<p>FLI If <math>FLI \geq 0</math>, all values of the flux table are initialized to the value FLI. If <math>FLI &lt; 0</math>, the flux array <math>\phi_{j,k}</math> is initialized to <math>e^{-(\sum_k)(x_j)}</math> FLI is usually set equal to zero. Next 8 columns.</p> <hr/> <p>W is an acceleration factor. If <math>\phi_{i+1}</math> is the flux computed on the <math>(i+1)</math>st iteration, <math>\phi_{i+1}</math> is replaced by <math>(W\phi_{i+1} + (1-W)\phi_i)</math>. If <math>w=1</math>, this procedure gives nothing new and the relationship is skipped. Next 8 columns.</p> <hr/> <p>XO. If <math>XO \geq 0</math> the left edge boundary of the flux array is initialized to the value of XO. If <math>X_0 &lt; 0</math> the left, or <math>X_0</math>, boundary fluxes are read in by input. Next 8 columns.</p> <hr/> <p>XN. If <math>XN \geq 0</math>, the right edge boundary of the flux array is initialized to the value of <math>X_N</math>. If <math>X_N &lt; 0</math> the right hand boundary fluxes are read in as input. Next 8 columns.</p>
4a	nuclide identification for region	24I3	<p>IELEW (I) I = 1,24 The nuclide identification numbers for all nuclides within the first spatial region are read in on a single card, in numerical order. These numbers correspond to nuclide data stored on tape NUTAPE, the nuclide data storage tape. Each entry occupies 3 columns. This table takes up n3 columns of one card, when n=number of nuclides within the region of computation</p>

Category No.	General Description	Format	Specific Input Quantity
4b	density of nuclides for a given region	9(E8.2)	DENSIT(I), the density (gms/cc) for each of the nuclides above. This pattern of a single card of IELEW data (4a category card) followed by the corresponding density card(s) (4b category card(s)) is maintained until all INONU regions of the problem have their composition defined. Each entry has 8 columns. This 4b table occupies a total of n8 columns, where n=number of nuclides within the region being computed.
5.	optional input. IDEBUG=20 indicates there is no nuclide data storage tape and we therefore read category 5 input.		
5a	IDEBUG is a category 2 indication	(E13.7, I6, I1)	ENZr, the energy corresponding to zero lethargy for the lethargy argument table of the cross-section data. This must be the maximum energy for the cross section table. First 13 columns floating point form. NOXSAG, the number of entries in the lethargy table corresponding to cross section input. Next 6 columns, fixed point. IBUG1, an indicator. Next column only. If IBUG1=1 we have constant cross sections. Therefore we read $\alpha_0, \alpha_1, \alpha_2, \alpha_4, \gamma_3, \gamma_4$ and $\gamma_5$ tables directly.

Category No.	General Description	Format	Specific Input Quantity
5a			Each of categories 5b, 5c, and 5e through 5l, require a table of numbers to be prepared for input. Each table entry is in floating point form where a number in the form $+ .ffffff \times 10^{+ee}$ is expressed $+ .ffffffE+ee$ . It is placed to the extreme right of the 13 column field reserved for it. One IBM input card can hold up to 4 entries. (65 columns).
5b		5(13.7)	XSLEAG (I)I= 1, NOXSAG, the table of lethargy arguments for all cross sections. See note following 5a, just above.
5c	Optional input: if IBUG1=1, we have constant cross section input. Therefore read Input 5. This option is valid only if there is 1 region.	5(E13.7)	<p>The following will form tables with constant values</p> <p>XSMATS(1) the total macroscopic cross section columns (1-13)</p> <p>ALFAO (1) value of <math>\alpha_0</math> columns(14-26)</p> <p>ALFA 1(1) value of <math>\alpha_1</math> columns(27-39)</p> <p>ALFA 2(1) value of <math>\alpha_2</math> columns(40-52)</p> <p>ALFA 3(1) value of <math>\alpha_3</math> columns(53-65)</p> <p>ALFA 4(1) value of <math>\alpha_4</math> columns(1-13) next card</p> <p>GAM 3(1) value of <math>\gamma_3</math> columns(14-26)</p> <p>GAM 4(1) value of <math>\gamma_4</math> columns(27-39)</p> <p>GAM 5(1) value of <math>\gamma_5</math> columns(40-52)</p> <p>XSEE 91) value of <math>\xi = C_{10}</math> (1) columns(53-65)</p>

Category No.	General Description	Format	Specific Input Quantity
5c	Optional Input. If IBUG1 $\neq$ 1, we have non-constant cross section input given in 5d-5e. This option permits arbitrary introduction of SPM coefficients without reference to NUTAPE tape.		
5d		I7,3A6, 2E15.6	NUCLNO, the identification number of the nuclide for which we are reading in cross section data columns (1-7) NAME, a 18 character title for this nuclide. Columns (8-25) AW, the atomic weight for this nuclide, columns (26-40) USQ, the quantity $\langle \mu \rangle$ columns (41-65)
5e		5E13.7	XSMIT(I) I=1, NOXSAG $\sigma_T$ , or microscopic total cross sections in barns See note following category 5a description.
5f		5E13.7	XSMIS (I) I=1, NOXSAG $\sigma_s$ , or microscopic scattering cross section in See note following 5a description.
5g		(5E13.7)	C10(I) I=1, NOXSAG SPM coefficient defined in text. See note following 5a description.
5h		(5E13.7)	C20(I) I=1, NOXSAG See note following 5a description.

Category No.	General Description	Format	Specific Input Quantity
5i		(5E13.7)	C02(I) I = 1, NOXSAG See note following 5a description
5j		(5E13.7)	C <sub>12</sub> (I) I = 1, NOXSAG See note following 5a description
5k		(5E13.7)	WV0(I) I = 1, NOXSAG See note following 5a description
5l		(5E13.7)	WV1(I) I = 1, NOXSAG See note following 5a description Note that if IDEBUG $\neq$ 20, all category 5 and 6 data are read from the nuclide data storage tape NUTAPE.
6	Optional Input. If ISOUR 1 = 0, read the lethargy = 0 source	(9E8.2)	FLUX(I) I = 1, J2 Fluxes at lethargy zero level, including corner points. J2 x 8 columns, with at most 9 entries on a card.
7	Optional Input. If D010 = 1, read in tables of arbitrary D <sub>10</sub> sources	(9E8.2)	FIST(I) Arbitrary D <sub>10</sub> sources. For each lethargy level from KBGIHS (category 2) to KIST (category 2), inclusive, J2 (category 2) values of D <sub>10 j,k</sub> will be read in, from x <sub>0</sub> to x <sub>N</sub> .  (KIST-KBGIHS+1) sets of (J2 x 8 columns)
8	Optional Input. If X <sub>0</sub> < 0 read in X <sub>0</sub> side boundary condition	(9E8.2)	FLUX(I) K2 entries of the left or X <sub>0</sub> boundary values of flux, starting from lethargy level K=1. (K2 x 8) columns
9	Optional Input If X <sub>N</sub> < 0, read in X <sub>N</sub> side boundary conditions	(9E8.2)	FLUX(I) K2 entries of the right or X <sub>N</sub> boundary values of flux, starting from lethargy level K=1.

## V. SPM Output

The SPM output of results is initiated by a printout of a) the names of nuclides, and b) their corresponding densities in nuclei/cm<sup>3</sup> in each successive region.

By a proper choice of the input indicators, IPCY and IMALP (category 2 input), the SPM program may be set up to print out convergence data, for each or any flux iteration number, in the following form:

Line 1: (flux iteration number), (number of points tested for convergence), (average residual), (maximum residual), (j position of max. residual (space)), (k position of max. residual (lethargy))

Line 2: (B1, Minimum Value of Flux), (B2, Maximum Value of Flux), (absolute value of maximum of (B2, -B1))

At iteration IMALP and at completion of the problem by either convergence or divergence, SPM prints out problem identification comments. SPM briefly prints out why the problem ended. It then prints the flux array requested by input indicators MKO and MJO (category 2 input). The energy level and space position identifying each element of the flux array is printed on each page.

## VI. GENUC - Cross Section Processing Program

### A. Purpose

The purpose of the GENUC program is to produce NUTAPE from microscopic cross section data. It produces also an edited version of NUTAPE for printing. A printed record is necessary for the operator to have in order to identify the various nuclides. The following data are given on NUTAPE for each nuclide.  $A$ ,  $\langle \mu^2 \rangle$ ,  $\sigma_T$ ,  $\sigma_S$ ,  $C_{10}$ ,  $C_{20}$ ,  $C_{02}$ ,  $C_{12}$ ,  $v_0$ , and  $v_1$ . GENUC has an option whereby  $C_{12}$  and  $v_1$  can be put equal to zero. This is equivalent to dropping the third-order terms. This option is denoted in the following by  $\gamma = 0$ .

All data thus collected for a given nuclide, along with title information, are written on tape as a single record, in the exact order SPM requires.

GENUC provides for the sequential storing of many nuclide-data records on the same tape. A necessary restriction of storage on one tape is that each nuclide must use the same table of lethargy arguments. The lethargy table and title information to identify this particular tape are found as the first record.

### B. Tape Unit Designations

GENUC consists of a main program and one subroutine CHANTP. Because of the organization of the subroutine CHANTP, the GENUC code, like the SPM program, may be run at any 7090 installation regardless of the standard input and output tape designations of that installation.



The GENUC code deck issued with this report uses the logical tape units listed in the table below.

<u>Unit</u>	<u>Use</u>
2	Input
3	Output, Hollerith
5	Output of nuclide-data, in binary form, for use with the SPM program

The procedure for changing the logical tape designations that GENUC uses is exactly the same as for the SPM code.

#### C. Input Preparation and Restrictions

An input deck for the preparation of a new data-storage tape (i.e. when the input quantity  $N\emptyset\emptyset NTP = 0$ ) must carry both a lethargy division table and its associated base energy for  $u = 0$ , both of which will be maintained as a standard for all successive lethargy-dependent variables on this tape. When  $N\emptyset\emptyset NTP > 0$ , the lethargy table will be assumed present within the first tape record and the input deck need only contain information directly related to the given nuclide. Any number,  $N\emptyset NUC$ , of different nuclides may be added to the tape, with two restrictions: 1) GENUC provides no interpolation facilities for non-standard lethargy arguments; and 2) the use of the  $\gamma$ - option (defining  $\gamma$  to be zero or non-zero) remains the same for all  $N\emptyset NUC$  nuclides. When the GENUC run is complete for these  $N\emptyset NUC$  records, the GENUC program starts anew. At this time for the new run, the  $\gamma$  option of course may be changed.

## GENUC DEFINITIONS

NØNUC	Number (Index maximum) of nuclides to be added onto data storage tape
NØØNTP	The actual number of nuclide records on the nuclide data tape. If 0, then we prepare a new nuclide tape.
IBUG	Indicator for $\gamma$ option When IBUG = 1, the tables C12(L) and WV1(L) are set equal to zero for all lethargies L.
XSLEAG(I)	Table of lethargy arguments for cross-section tables with a NØXSAG number of entries.
NØXSAG	The number of entries to above table, $\leq 200$ .
NIDTAP	A label, or title, to be printed out for identification of a particular nuclide data tape
ENZR	The base energy for which lethargy is defined as zero
NUCLNØ	Number-label of a nuclide
NAME	18 Alpha-numeric character (3 cell) title for a nuclide
AW	Atomic weight of the nuclide
USQ	$\langle \mu^2 \rangle$
FL(KK,L)	Legendre coefficients $f_\ell$ for the nuclide. Here KK = $\ell + 1$ There are 7 separate such tables for KK = 2 to KK = 8 L is the lethargy index Each such table has NØXSAG entries in it, corresponding to the XSLEAG table of arguments
XSMIT(L)	Microscopic cross-section in barns corresponding to XSLEAG lethargy table, NØXSAG entries
XSMIS(L)	Microscopic cross-section in barns corresponding to XSLEAG lethargy argument table, NØXSAG entries

**Input to GENUC consists of the following sets of cards. Refer to GENUC Definitions.**

Card Set Identification Number	No. of Cards*	When Needed	Card Columns										Mode	Format		
G1	1	Each Problem	1	3	4	6	7	9					72	All Fixed	2413	
			1	NOXUC		NOXNTP		YBUG								
G2	1	Only When NOXNTP = 0	1	3	4	NOXSAG (≤ 200)			6					72	All Fixed	
			1	NYDTAP												
G3	$\left( \frac{NOXAG+1}{5} \right)$	Only When NOXNTP = 0	*1	13	14	26	27	39	40	52	53	65		All Floating	5E13.7	
			1	XSLEAG(1)		XSLEAG(2)		XSLEAG(3)		XSLEAG(4)		XSLEAG(5)				
			1	XSLEAG(6)		.....		XSLEAG(NOXNTP)		ENZR						
			After NOXSAG entries of XSLEAG, ENZR is punched													
G4	1	Each Problem	1	7	8	NAME, any 18 punchable characters				25	26	40	41	55	Fixed; any punchable characters; Floating, Floating	17, 3A6, 2E15.6
			1	NUCLNO						AW		USQ				

The following card sets G5 through G7 are repeated  $\text{NONUC}$  times, i.e. one set per nuclide.

Card Set Identification Number	No. of Cards*	When Needed	Card Columns											Mode	Format	
G5	$\left\{ \frac{\text{NOXSAG}}{5} \right\}$	Each Nuclide	*1 FL(KK,1) 1 FL(KK,6)	13 14 ...	26 FL(KK,2) ...	27 FL(KK,3) FL(KK,NOXSAG)	39 FL(KK,3) FL(KK,NOXSAG)	40 FL(KK,4) FL(KK,NOXSAG)	52 FL(KK,4) FL(KK,NOXSAG)	53 FL(KK,5) FL(KK,NOXSAG)	65 FL(KK,5) FL(KK,NOXSAG)	This table of Legendre coefficients is repeated for a total of 7 distinct tables, KK = 2 to KK = 8.			All Floating	5E13.7
G6	$\left\{ \frac{\text{NOXSAG}}{5} \right\}$	Each Nuclide	*1 XSMT(1) 1 XSMT(6)	13 14 ....	26 XSMT(2) ....	27 XSMT(3) XSMT(NOXSAG)	39 XSMT(3) XSMT(NOXSAG)	40 XSMT(4) XSMT(NOXSAG)	52 XSMT(4) XSMT(NOXSAG)	53 XSMT(5) XSMT(NOXSAG)	65 XSMT(5) XSMT(NOXSAG)				All Floating	5E13.7
G7	$\left\{ \frac{\text{NOXSAG}}{5} \right\}$	Each Nuclide	*1 XSMIS(1) 1 XSMIS(6)	13 14 ...	26 XSMIS(2) ...	27 XSMIS(3) XSMIS(NOXSAG)	39 XSMIS(3) XSMIS(NOXSAG)	40 XSMIS(4) XSMIS(NOXSAG)	52 XSMIS(4) XSMIS(NOXSAG)	53 XSMIS(5) XSMIS(NOXSAG)	65 XSMIS(5) XSMIS(NOXSAG)				All Floating	5E13.7

Return to directions for G5 input set until  $\text{NONUC}$  number of nuclides are punched.

\* The notation  $\{x\}$  means the least integer  $\geq x$ . A starred entry requires that a table continue on successive cards until NOXSAG entries have been punched.

## OUTPUT OF GENUC PROGRAM

The First Record has

NIDTAP

NOXSAG

XSLEAG(I), I = 1, NOXSAG

Each successive record describes a distinct nuclide and contains:

NUCLNØ

NAME 18 characters

AW atomic weight

XSMIT(L)  $\sigma_T$

XSMIS(L)  $\sigma$  scattering

C10(L) (Note that  $\xi$ , defined in SPM text, is

C20(L) never distinct from  $C_{10}(1)$ )

C02(L)

\* C12(L)

VO(L)

\* V1(L)

end of record

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\* We note that where IBUG = 1 (G1 input), the C12(L) and also the V1(L) tables will be set equal to zero.

### REFERENCES

1. C.N. Klahr and H.J. Zell, "The SPM (Stochastic Process Method) Equation for Calculating the Spatial Variation of Neutron Spectra", WADD-TR-60-312 (September, 1960).
2. H. Kaper, unpublished manuscript.

<p> Aeronautical Systems Division, Dir/Materials  and Processes, Physics Lab, Wright-Patterson  AFB, Ohio.  Rpt Nr ASD-TDR-63-89. THE SPM METHOD FOR  NEUTRONS. Final report, Mar 63, 64p. incl  tables, 2 refs. </p> <p> Unclassified Report </p> <p> The SPM equation has been recoded for the  IBM-7090. Both theoretical analysis and  some numerical results are given and dis-  cussed. </p> <p> ( over ) </p>	<p> 1. Difference equa-  tions  Neutrons  AFSC Project 7360,  Task 736003  Contract AF 33  (616)-7732  TRG, Inc.  Syosset, New York  R. Aronson,  J. Heitner  Secondary Rpt No.  TRG-149-FR  Aval fr OTS  In ASTIA collec-  tion </p>	<p> 1. Difference equa-  tions  Neutrons  AFSC Project 7360,  Task 736003  Contract AF 33  (616)-7732  TRG, Inc.  Syosset, New York  R. Aronson,  J. Heitner  Secondary Rpt No.  TRG-149-FR  Aval fr OTS  In ASTIA collec-  tion </p>	<p> 1. Difference equa-  tions  Neutrons  AFSC Project 7360,  Task 736003  Contract AF 33  (616)-7732  TRG, Inc.  Syosset, New York  R. Aronson,  J. Heitner  Secondary Rpt No.  TRG-149-FR  Aval fr OTS  In ASTIA collec-  tion </p>